

**SYLLABUS Physical Chemistry 320-334:
INTRODUCTION TO QUANTUM CHEMISTRY AND
SPECTROSCOPY**

Chemistry 320-334, Spring 2008
NSC 210, Tu, Th, 09.30 – 10.50.

Instructor: Dr. P. Coppens

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Office Hours: NSC732, 2-3pm Tuesday; 12-1pm Thursday, or by appointment. An appointment can be made by e-mail to coppens@buffalo.edu. *For personal communication, office hours are preferred to e-mail*

Teaching Assistant: to be assigned. Office hours to be announced.

Text: Physical Chemistry 7th Edition by Peter Atkins and Julio de Paulo (W. H. Freeman & Co. NY). A student solutions manual is available with worked out solutions for half of the problems in the text.

The course will highlight how quantum mechanical concepts are needed to understand modern Chemistry, including the electronic structure of atoms, how atoms are linked into a molecule by chemical bonds, how molecules react to light, how lasers work, magnetic resonance. The course will include hands-on theoretical calculations of simple molecules.

Note: This course requires regular class attendance and reading to prepare for the lectures.

Grading:

Midterm 1, 100 points

Midterm 2, 100 points,

Final Exam, 150 points,

Quizzes (2 or 3) ~25 points each

Participation in class: 10% of total score.

The following topics will be covered:

- Basic principles of Quantum Theory as relevant to Chemistry (Chapter 11)
- Methods and application of Quantum Chemistry (Chapter 12).
- The concept of atomic orbitals and their description by quantum numbers. The interpretation of quantum numbers (Chapter 13).
- Bonding in simple molecules, molecular structure (Chapter 14).
- Vibrational and Electronic spectroscopy, Lasers (Chapters 16 and 17).
- Introduction to Magnetic Resonance (Chapter 18)

What is expected from you:

- regular class attendance
- reading of the relevant sections of the text book to understand rather than memorize the material.
- ***doing the homework***